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OBSERVATION OF HIGH FIELD DHVA-EFFECT AND INDUCED MAGNETISM IN SINGLE CRYSTAL $TiBe_2$

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1. Introduction

Recently much interest has been given to itinerant magnetism in cubic Laves phase or C15 materials. Primarily this stems from the discussion [1] of the relationship of p-state pairing and ferromagnetism in $ZrZn_2$ by Enz and Matthias, and the possibility of triplet superconductivity [2]. The most recent work in this field has focused [3] on the isoelectronic, isostructural material $TiBe_2$, and the possibility that this material is metamagnetic [4]. That $TiBe_2$ is close to some form of magnetic instability can be inferred indirectly from the peaked nature of its density of states [5, 6] near the Fermi level, but also from the observation of ferromagnetism [7, 8] in $TiBe_{2-x}Cu_x$, when x is greater than about 0.15. In this paper we consider a single crystal of pure $TiBe_2$ in fields larger than 15 T and at a temperature of 1.3 K.

2. DHVA experiment

The material used in these experiments has been prepared by arc-melting. From this material a single crystal grain has been selected, whose size was about 1.0; 0.5; 0.5 mm and whose axis was along a [110] direction. A series of Laue photographs showed that the sample was a coherent single crystal with only minor inclusions. The DHVA spectra were recorded using the same equipment as for an earlier study on polycrystalline $TiBe_2$ [9]. Distinct DHVA-frequencies were observed for many different orientations at fields larger than 15 T. In order to improve the signal to noise ratio the average was taken over several runs.

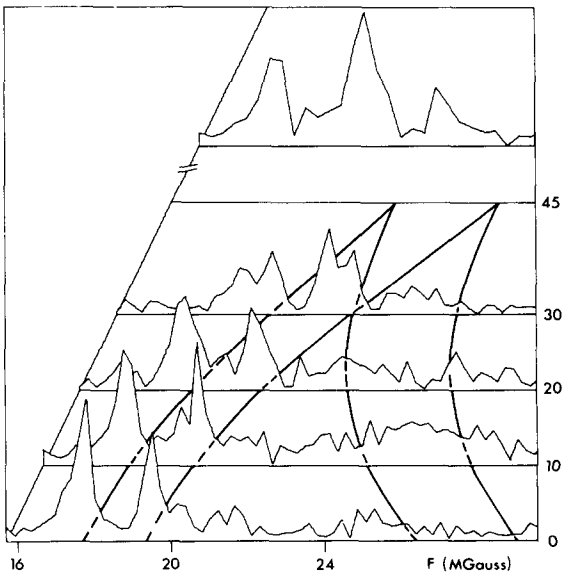

Fig. 1. Angular dependence of the $TiBe_2$ DHVA spectra from [110] toward [100]. The heavy lines are from a $\boldsymbol{k} \cdot \boldsymbol{p}$ X_7 theoretical model, whose splitting was 2.6 mRy. The upper insert shows the polycrystalline data from ref. 9. As discussed in the text, these data show that $TiBe_2$ is in a ferromagnetic state in fields above 15 T.

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All observed spectra were similar. The dominant common feature was the observation of two nearly equal frequency peaks, separated by about 200 T. Direct plots of these spectra spaced by 10° in the (001) plane are shown in fig. 1. The observed frequencies varied by about 10% and assumed minimal values – 1800 and 2000 T – at [110]. These values are the same as those observed in the polycrystalline experiment [9]. The amplitudes for the various angles can be intercompared and follow the orbital cyclotron mass approximately. The cyclotron mass of both [110] frequencies was 1.3 ± 0.2. Using the band orbital mass of 0.51, we find a λ of 1.5 or about *one-half* of the specific heat derived λ of 3.1 [5].

3. Bandstructure

In this study we have added the effects of the non-spherical parts of the potential *within* a Ti muffin-tin sphere radius, to the outside or warped corrections included previously [5]. Such corrections are small since they result from the broken T_d symmetry of the inside deviations in this most close-packed lattice. Their net effect is to shift downward $\Gamma_{25'}$ or T_{2g} symmetry derived structure by about 7.4 mRy relative to Γ_{12} or E_g symmetry structure. The effect can be simply understood in that the inside Ti potential deviations are *deeper* in T_d symmetry when looking in the [111] direction than [100], and that band states of $\Gamma_{25'}$ derived structure more dominantly lie along [111] than [100]. The resultant paramagnetic $TiBe_2$ Fermi surface shows only microscopic deviations from de Groot et al. [5], since the density of states near E_F is made up mostly from T_{2g} orbitals. Near E_F, band 7, whose importance will become clear below, is made up almost entirely from E_g symmetry except along the critical X to W line where band 7 is mainly T_{2g}. The net effect is that band 7 loses 0.023 electrons to bands 8, 9 and 10, when inside potential corrections are included.

4. Possible metamagnetism in $TiBe_2$

The extremal cross-sections shown as heavy lines in fig. 1 were derived from band 7, by applying a rigid splitting of the Fermi surface into spin up and spin down subsheets to a quadratic $\boldsymbol{k} \cdot \boldsymbol{p}$ Hamiltonian fitted near X to the ab initio points near X. The r.m.s. accuracy was better than 0.2 mRy. The separation corresponds to $0.11\,\mu_B$ or 2.6 mRy [10]. This same band 7 sheet occurs in the same way in Jarlborg and Freeman [6]. We can apply rigidly this splitting – 2.6 mRy – to *all* bands, as being representative of $TiBe_2$ when subject to fields stronger than 15 T. The effect on the Fermi surface is shown in fig. 2. These plots were made by selecting from 10 000 random points those whose energy was within 0.5 mRy of E_F. The band 7 sheet appears with low density because of its small (0.51) mass, whereas bands 8 and 9 are quite dense.

Noteworthy is the opening up of the jungle gym of band 8 in the minority sheet in the (001) plane, and of band 9 in the majority sheet in the (110) plane near L. Such effects arise, of course, as a consequence of the confluence of van Hove singularities with E_F. Note that the "hottest" or heaviest sheets dominantly have confluence in $TiBe_2$. Remarkably, the same effect appears in a recent theoretical discussion of Jarlborg and Freeman [11] on metamagnetism in Pd above 300 T.

Magnetism implies a metastable induced ferromagnetic state. Although the conditions discussed by Wohlfarth and Rhodes [4] as necessary for metamagnetism are present in our theoretical model of $TiBe_2$, we can only claim here that our experiments show induced magnetism, since we have not tested explicitly metastability. We do believe it likely that $TiBe_2$ has a metamagnetic phase. The clearest possible support for this conjecture might emerge from a search for the time dependence of the (ferro)magnetic moment distribution of $TiBe_2$ when placed in a magnetic field of about 15 T. The results should resemble $ZrZn_2$ [12] or $TiBe_{2-x}Cu_x$ [8] initially, and then decay away.

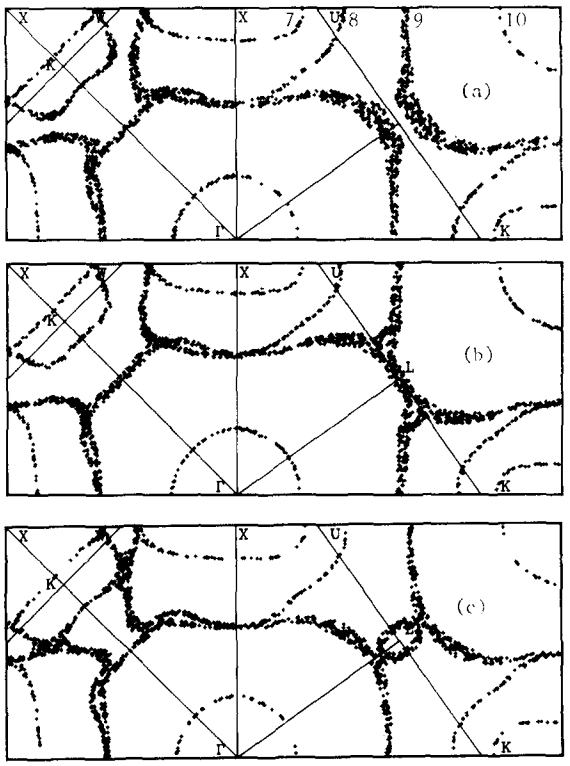

Fig. 2. Theoretical Fermi surface for paramagnetic $TiBe_2$ (a) and for ferromagnetic majority (b) and minority (c) spin directions, respectively. The confluence of van Hove singularities near L in the majority band 9 sheet and around K for the minority band 8 sheet strongly suggests metamagnetism in $TiBe_2$.

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